

**Computational Design and Prototype Evaluation of Aluminide-Strengthened Ferritic Superalloys for Power-Generating Turbine Applications up to 1,033 K**

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## ABSTRACT

In this joint university endeavor among The University of Tennessee, Northwestern University, and The University of California, Davis, a computer-aided alloy-design approach is proposed to optimize the development of high-temperature materials through (i) utilizing high-performance computations and simulations to identify prototype alloy compositions and heat treatments and (ii) employing a wide range of experimental techniques to synthesize, characterize, and gauge the properties of the prototype alloys. Northwestern University and The University of California, Davis, will collaborate in conducting the first-principles calculations to develop reliable multicomponent thermodynamic and kinetic databases for the alloy design. The University of Tennessee will lead the efforts in the alloy fabrication, mechanical-property studies, and oxidation/corrosion investigations. Both Northwestern University and The University of Tennessee will also collaborate in microstructural characterizations (e.g., using scanning-electron microscopy, conventional transmission-electron microscopy, high-resolution analytical-electron microscopy, and X-ray diffraction).

The objective of this proposal is to integrate modern computational tools with focused experiments to design innovative ferritic superalloys strengthened mainly by the NiAl-type (*B2*) phase for fossil-energy applications up to 1,033 K. First-principles-based calculations will be performed to predict the phase stability of equilibrium phases in the Fe-Al-Cr-Ni system. The first-principles calculations will be incorporated in a *Thermo-Calc* database. A comprehensive mobility database for the body-centered cubic and *B2* phases will be developed to simulate the kinetics of diffusional transformations. The composition trajectory and coarsening process of nanoscale *B2* precipitates in multi-component Fe-based alloys will be predicted by including capillarity and the effective strain energy of a two-phase coherent mixture in the computational thermodynamic and kinetic models. Theoretical predictions of microstructures will be verified by the fabrication and microstructural analyses of the prototype alloys. These alloys (or modified alloys, if necessary) will be studied for their creep behavior and oxidation/corrosion resistances with respect to the design target. Specifically, the computational alloy/microstructural design aims to achieve a steady-state creep rate of approximately  $10^{-11} \text{ s}^{-1}$  at a temperature of 1,033 K and a stress level of 35 MPa.

Innovative high-temperature materials are critical in improving the efficiency and lowering the emissions of advanced turbine-power-generation systems and enabling the development of new power-generation systems. The traditional trial-and-error approach to the development of new materials has proved to be too sluggish to keep pace with aggressive standards. For example, the Ultra-Supercritical Steam Turbines Program sponsored by the Department of Energy (DOE) Fossil Energy Program requires the increase of the steam temperature from 866 to 950 K by the year of 2010 and to 1,033 K by 2020. The current proposal will advance the development of computational models for the accelerated design of high-temperature ferritic steel materials. The outcomes of the present work will include (i) the development of a new high-temperature, creep-resistant class of ferritic “superalloy” steels for applications in advanced coal-based energy systems and (ii) the establishment of robust validated databases for the elevated-temperature alloy design.